Idaho National Laboratory

A Multi-Physics Simulation Capability at the INL for High-Resolution Analysis of Reactor Systems

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Abstract

The Idaho National Laboratory (INL) has embarked on a extensive research project to develop a unified multi-physics algorithm and construct a three-dimensional pilot code to model the gas-cooled Generation IV reactor and specific components in a high-resolution manner. Designed for deployment on massively parallel computing platforms, this pilot program will simulate advanced reactor behavior with spatial resolution and completeness of detailed physics unparalleled in previous reactor simulation experience. Through the *unifying principle of energy conservation*, all reactor structures and materials (fuel, moderator, coolant, and structural components) will be modeled with a single continuous mesh representation over which radiation, mass, and energy transport will be simultaneously solved. This unified physics approach to simulating Generation IV reactor technology requires fewer simplifying assumptions and approximations and will ultimately result in accuracy levels far exceeding previous efforts. Once completed, this unique simulation tool will allow many reactor designs and modifications (optimizations) to be analyzed with unprecedented detail at minimal cost for both normal operation and accident scenarios. Such analytical power will greatly reduce the need for extensive prototyping.

Overview of Presentation Topics

1. Statement of Research
2. Collaborators
3. Basic Approach
4. Unified Multi-Physics Algorithm
   - Governing Equations
   - PCICE-FEM Scheme
   - EVENT Transport Code
   - Coupling Procedure
   - Simplified Multi-Phase Approach (PBR)
5. Tasks
6. Questions and Advice

Research Goal: This research is specifically focused on developing a multi-physics algorithm and constructing a three-dimensional pilot code to simulate the thermal behavior of the gas-cooled Generation IV reactor concept in a high-resolution manner, both in terms of spatial resolution and completeness of detailed physics.

- All reactor structures and materials (fuel, moderator, and structural components) will be modeled with a single continuous mesh representation over which radiation, mass, and energy transport will be solved.
- Designed for deployment on massively parallel computing platforms
- The unified physics approach to simulating Generation IV reactor technology requires fewer simplifying assumptions and approximations and will ultimately result in accuracy levels far exceeding previous efforts.
- Will allow many reactor designs and modifications (optimizations) to be analyzed with unprecedented detail at minimal cost for both normal operation and accident scenarios. Thus, the need for extensive prototyping will be greatly reduced.

Project Collaborators:

1. Idaho National Laboratory (Fission and Fusion Systems Department)
   - Project lead
   - Coupled CFD and solid phase heat transfer (PCICE)
2. Argonne National Laboratory (Mathematics and Computer Science Division)
   - HPC computing (MPI, PETSc, Sieve Data Structure)
   - Mesh management (parallel mesh generation, domain decomposition, AMR)
3. Georgia Institute of Technology (George Woodruff School of Mechanical Engineering)
   - Radiation transport (EVENT)

Basic Approach

- Strong mathematical coupling of governing physics (multi-physics)
- Consistent Spatial and Temporal Discretization (address conflicting space and time scales)
- High-Resolution of all Relevant Physics (turbulent BLs, strong pressure and temperature gradients/transients, radiation transport)
- Deployed on HPC platform (OZONE)
- Validation (combined small-scale experiments, analytical and known benchmarks)

Governing Equations:

Mass

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \rho \vec{u} = 0$$

Momentum

$$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla} \cdot \left(\rho \vec{u} \otimes \vec{u} \right) = -\vec{\nabla} P + \vec{\nabla} \cdot \underline{\tau}$$

EOS $P = f(\rho, e)$

Total Energy

$$\frac{\partial \rho e_t}{\partial t} + \vec{\nabla} \cdot \rho \vec{u} H = \vec{\nabla} \cdot \left(\underline{\tau} \cdot \vec{u} \right) + \vec{\nabla} \cdot \left(k \vec{\nabla} T \right) + i$$

Neutral-Particle

$$\frac{1}{v} \frac{\partial \varphi(\vec{r}, \vec{\Omega}, E, t)}{\partial t} + \vec{\Omega} \cdot \vec{\nabla} \varphi(\vec{r}, \vec{\Omega}, E, t) + H \varphi(\vec{r}, \vec{\Omega}, E, t) = S(\vec{r}, \vec{\Omega}, E, t)$$

PCICE-FEM* Scheme

- Pressure-Corrected Implicit Continuous-fluid Eulerian (PCICE) algorithm is combined with the Finite Element Method (FEM)
- Developed for "All-Speed" (nearly incompressible to highly compressible)
- Fractional-Step (non-iterative)
  1. Explicit Predictor (neglect pressure and source terms)
  2. Implicit Diffusion (viscous and thermal plus sources)
  3. Pressure Poisson (implicit pressure)
  4. Semi-implicit Pressure Correction (pressure effects)

* R.C. Martineau and R.A. Berry, "The pressure-corrected ICE finite element method for compressible flows on unstructured meshes," Journal of Computational Physics, Vol. 198, p. 659, 2004.

Hydrodynamic Temporal Discretization

Mass

$$\rho^{n+1} = \rho^{n} - \Delta t \vec{\nabla} \cdot \left[\theta \left(\rho \vec{u} \right)^{n+1} + \left(1 - \theta \right) \left(\rho \vec{u} \right)^{n} \right]$$

Momentum

$$\left(\rho \vec{u} \right)^{n+1} = \left(\rho \vec{u} \right)^{n} - \Delta t \vec{\nabla} \cdot \left(\rho \vec{u} \otimes \vec{u} \right)^{n+\theta} - \Delta t \vec{\nabla} \left[\theta P^{n+1} + \left(1 - \theta \right) P^{n} \right] + \Delta t \vec{\nabla} \cdot \underline{\tau}^{n+\theta}$$

Total Energy

$$\begin{aligned} \left(\rho e_{t} \right)^{n+1} = {} & \left(\rho e_{t} \right)^{n} - \Delta t \vec{\nabla} \cdot \left[\theta \left(\rho \vec{u} \right)^{n+1} H^{n+1} + \left(1 - \theta \right) \left(\rho \vec{u} \right)^{n} H^{n} \right] \\ & + \Delta t \vec{\nabla} \cdot \left(\underline{\tau} \cdot \vec{u} \right)^{n+\theta} + \Delta t \vec{\nabla} \cdot k \vec{\nabla} \left[\theta T^{n+1} + \left(1 - \theta \right) T^{n} \right] + \Delta t \, i^{n+\theta} \end{aligned}$$

Explicit Predictor

- *Momentum*

$$\left(\rho\vec{u}\right)^{*}=\left(\rho\vec{u}\right)^{n}-\Delta t\vec{\nabla}\cdot\left(\rho\vec{u}\otimes\vec{u}\right)^{n+\theta}$$

- *Mass*

$$\rho^{*}=\rho^{n}-\Delta t\vec{\nabla}\cdot\left[\theta\left(\rho\vec{u}\right)^{*}+(1-\theta)\left(\rho\vec{u}\right)^{n}\right]$$

- *Total Energy*

$$\left(\rho e_{t}\right)^{*}=\left(\rho e_{t}\right)^{n}-\Delta t\vec{\nabla}\cdot\left[\theta\left(\rho\vec{u}\right)^{*}+(1-\theta)\left(\rho\vec{u}\right)^{n}\right]H^{n}$$

Implicit Diffusion (viscous and thermal)

$$\left(1-\theta\Delta t\vec{\nabla}\cdot\frac{\partial\vec{F}_{v}^{imp}}{\partial U}\right)U'=\Delta t\vec{\nabla}\cdot\left[\theta\vec{F}_{v}^{*}+(1-\theta)\vec{F}_{v}^{n}\right]+\Delta tQ\,,\qquad U'=\bar{U}-U^{*}$$

Pressure Poisson:

$$\frac{1}{(\gamma-1)e^{n+\theta}}\left(p^{n+1}-p^{n}\right)-\theta^{2}\Delta t^{2}\vec{\nabla}\cdot\vec{\nabla}\left(P^{n+1}-P^{n}\right)=\left(\bar{e}-e^{n}\right)\left(\frac{\rho}{e}\right)^{n+\theta}+\theta^{2}\Delta t^{2}\vec{\nabla}\cdot\vec{\nabla}P^{n}$$

$$-\Delta t\vec{\nabla}\cdot\left[\theta\left(\overline{\rho\vec{u}}\right)+(1-\theta)\left(\rho\vec{u}\right)^{n}\right]$$

Pressure Correction:

- *Momentum*

$$\left(\rho\vec{u}\right)^{n+1}=\left(\overline{\rho\vec{u}}\right)-\Delta t\vec{\nabla}\left[\theta P^{n+1}+(1-\theta)P^{n}\right]$$

- *Mass*

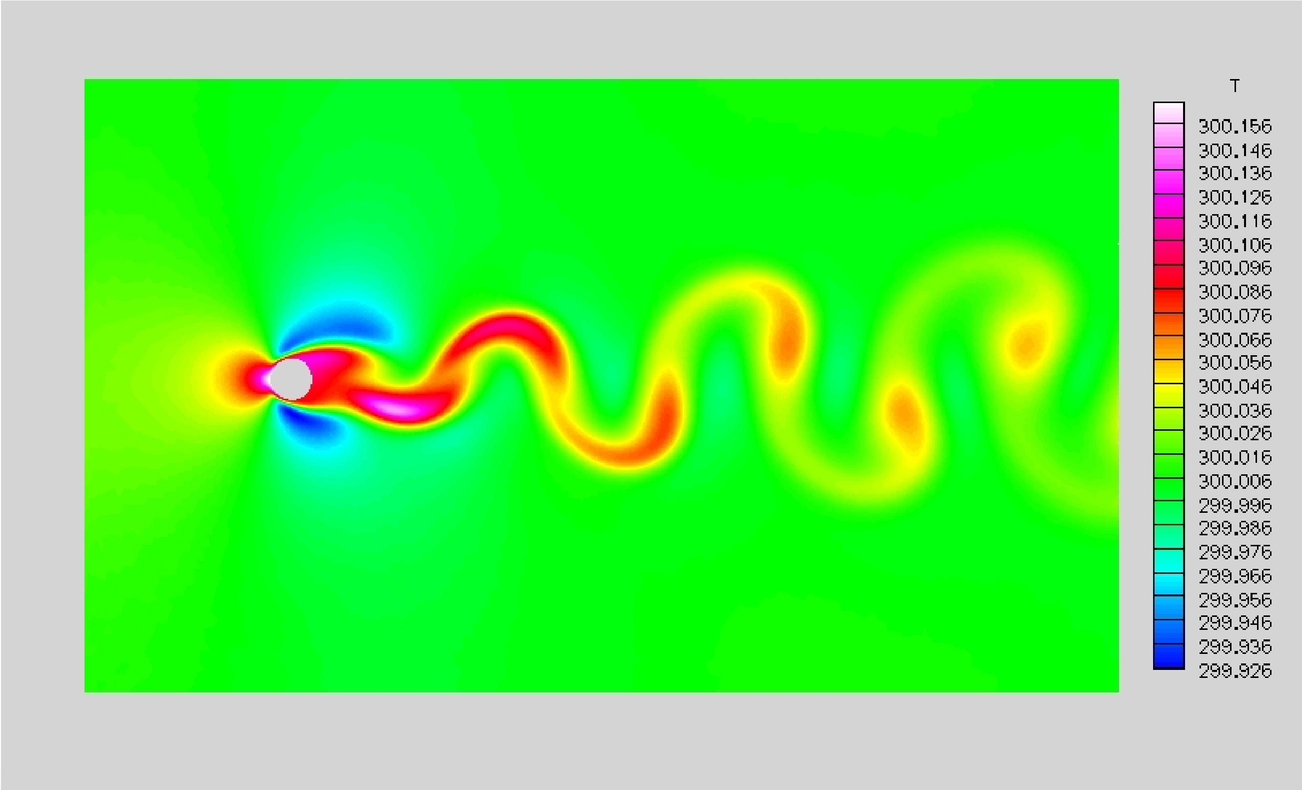
$$\rho^{n+1}=\bar{\rho}-\theta\Delta t\vec{\nabla}\cdot\left[\left(\rho\vec{u}\right)^{n+1}-\left(\overline{\rho\vec{u}}\right)\right]$$

- *Total Energy*

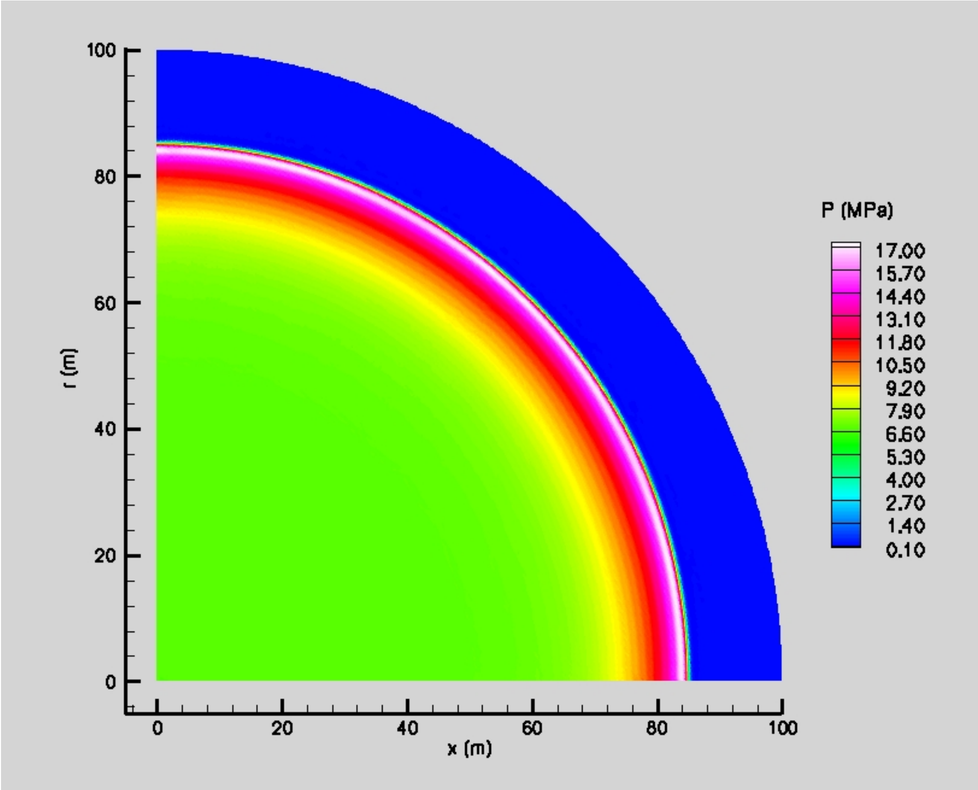
$$\left(\rho e_{t}\right)^{n+1}=\overline{\rho e_{t}}-\theta\Delta t\vec{\nabla}\cdot\left[\left(\rho\vec{u}\right)^{n+1}H^{n+1}-\left(\overline{\rho\vec{u}}\right)H^{n}\right]\qquad H^{n+1}=\frac{\overline{\rho e_{t}}+P^{n+1}}{\rho^{n+1}}$$

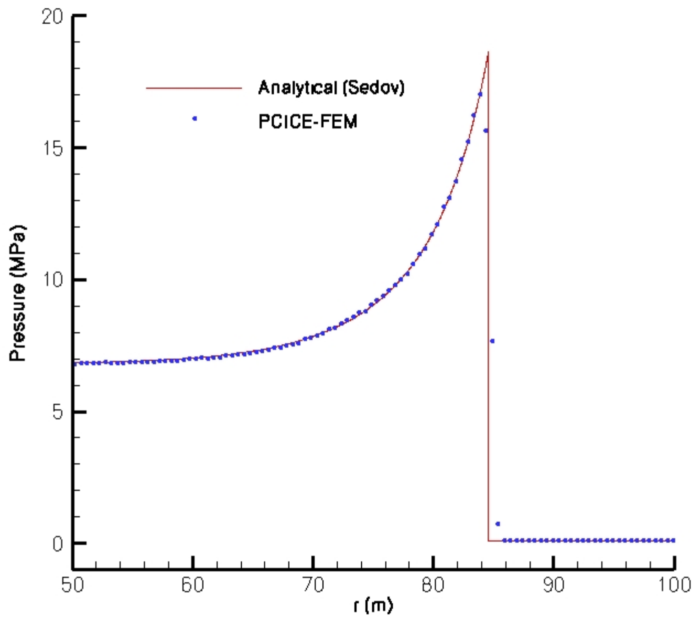
PCICE-FEM Simulation Examples

1) Von Karman Vortex Street (*Mach* = 0.05, *Re* = 100)



2) Intense Spherical Explosion (*Sedov Blast Wave*)





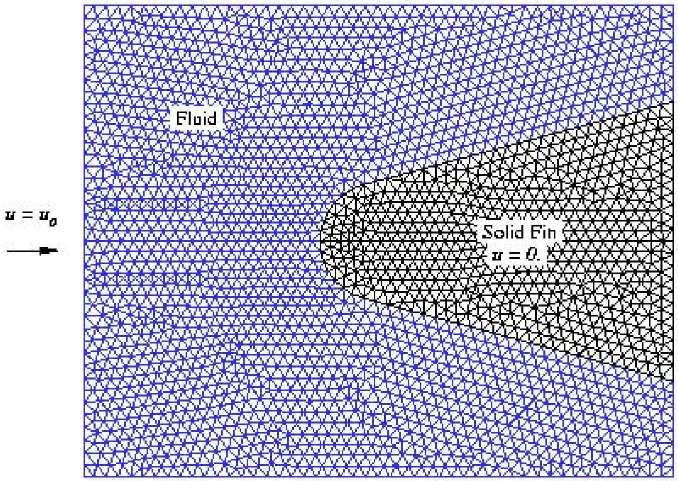
Initial Conditions => 1945 Trinity energy release, 7.19×10^{13} J. Solution shown at time $t = 8.0 \times 10^{-3}$ s.

EVENT Radiation Transport Code

- Even-Parity Neutral Particle Transport
- 3-D arbitrary geometry
- Time-dependent, steady-state and criticality modeling
- Multi-energy group approximation
- Finite Element (space)-Spherical Harmonics (angle) variational solution
- CFD coupling for criticality excursions
- Parallel implementation

Multi-Physics Coupling Procedure

Solid – Fluid Coupling



Full equation governing thermodynamic energy

$$(\rho e_t)^{n+1} - (\rho e_t)^{n} = -\Delta t \vec{\nabla} \cdot \left[\theta (\rho \vec{u})^{n+1} H^{n+1} + (1-\theta)(\rho \vec{u})^{n} H^{n} \right]$$
$$+ \Delta t \vec{\nabla} \cdot (\underline{\tau} \cdot \vec{u})^{n+\theta} + \Delta t \vec{\nabla} \cdot k \vec{\nabla} \left[\theta T^{n+1} + (1-\theta) T^{n} \right] + \Delta t\, i \left(T^{n+\theta} \right)$$

Reduces to heat conduction equation in solid

$$\rho C (T^{n+1} - T^{n}) = \Delta t \vec{\nabla} \cdot k \vec{\nabla} \left[\theta T^{n+1} + (1-\theta) T^{n} \right] + \Delta t\, i^{n+\theta}$$

Radiation Transport Coupling

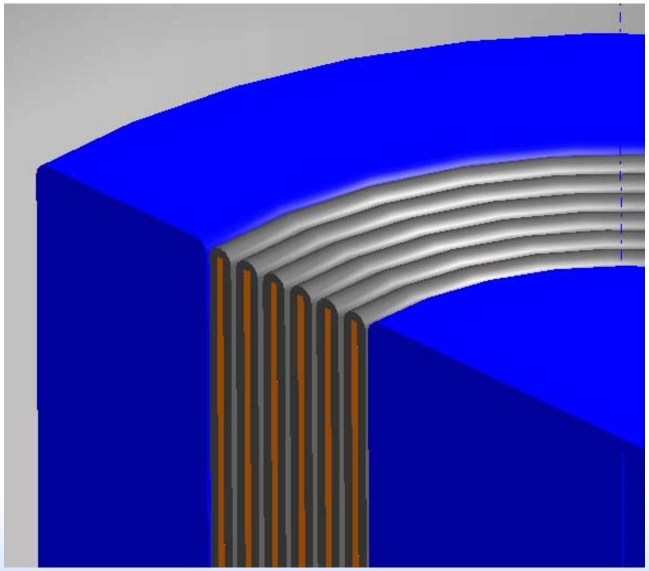
$$i = f(\vec{r}, T^{n+\theta}) = \int_{4\pi} d\vec{\Omega} \Sigma_f (\vec{\mathbf{r}}) \varphi(\vec{\mathbf{r}}, \vec{\Omega})$$ Spatially-dependent heat source due to fission

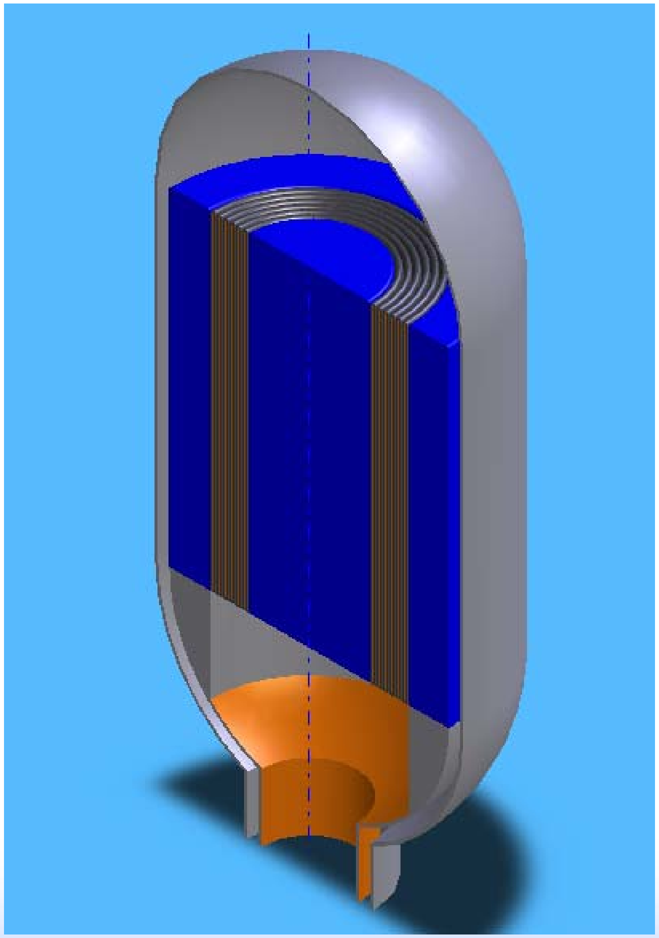
$$H \rightarrow H(T^{n+\theta})$$ Temperature feedback to material cross-section properties

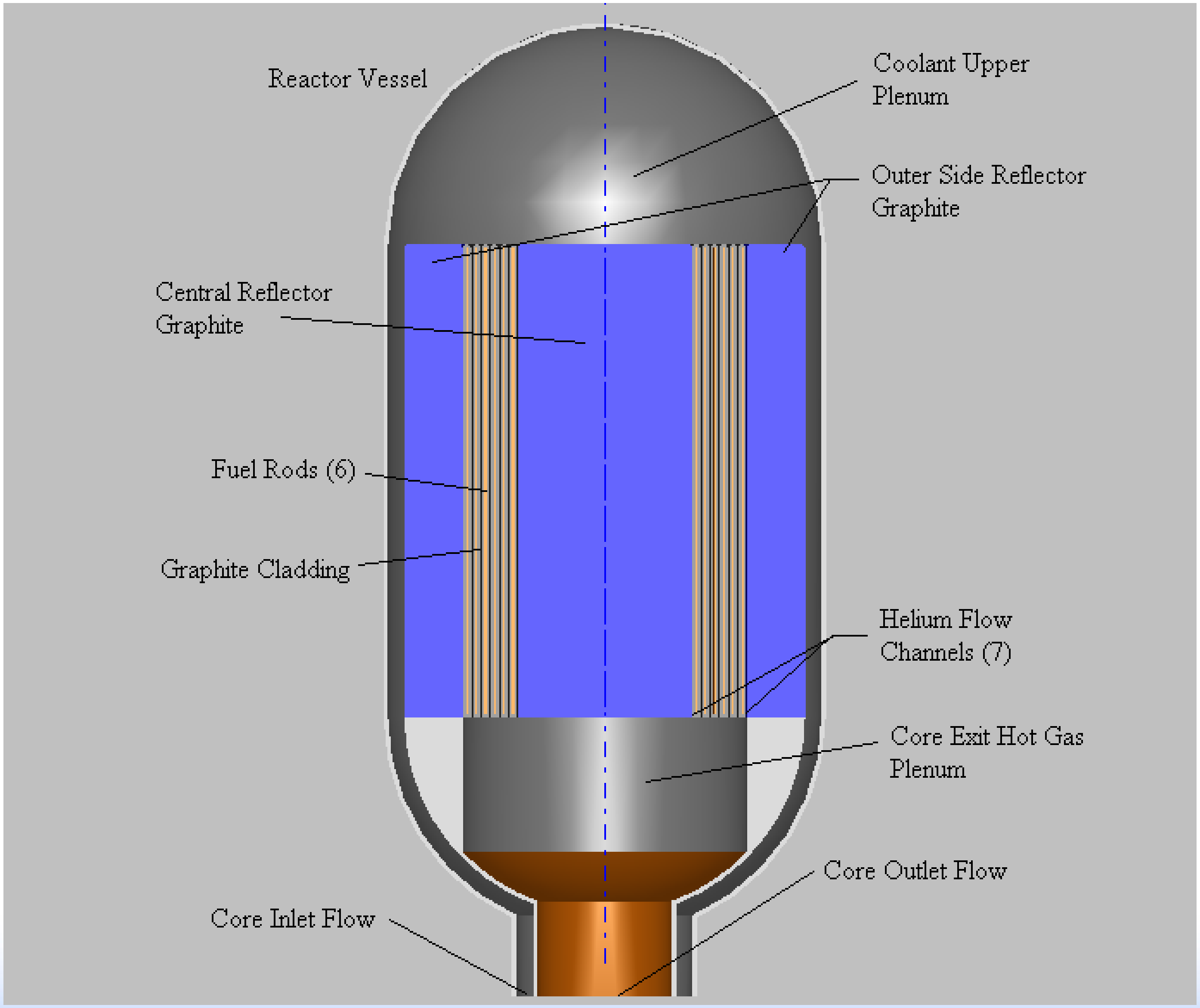
Tasks

1. Two-Dimensional Algorithmic Demonstration

- 2-D axisymmetric (*r, z*) geometry.
- Full coupling of solid-state and hydrodynamic heat transfer (PCICE) with and nuclear heating (EVENT).
- Ideal simulation of rapid LOCA.






Reactor Vessel
Coolant Upper Plenum
Outer Side Reflector Graphite
Central Reflector Graphite
Fuel Rods (6)
Graphite Cladding
Helium Flow Channels (7)
Core Exit Hot Gas Plenum
Core Outlet Flow
Core Inlet Flow

Simple Pebble-Bed Model*

- **Mass**

$$\frac{\partial \alpha \rho_g}{\partial t} + \vec{\nabla} \cdot \alpha \rho_g \vec{u}_g = 0$$

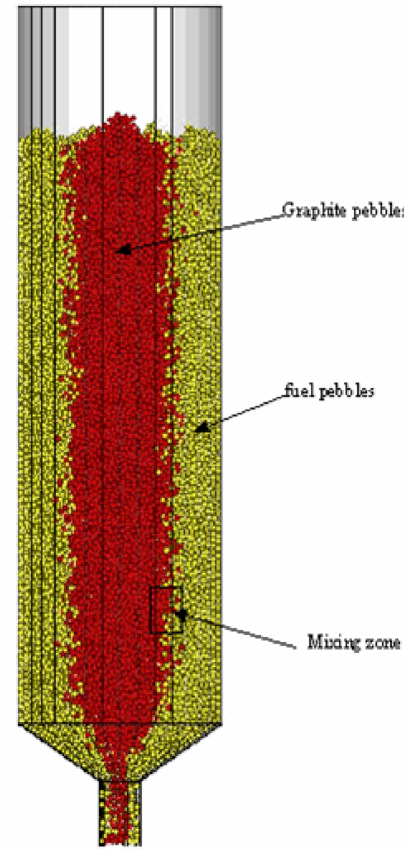
- **Momentum**

$$\frac{\partial \alpha \rho_g \vec{u}_g}{\partial t} + \vec{\nabla} \cdot \left(\alpha \rho_g \vec{u}_g \otimes \vec{u}_g \right) + \vec{\nabla} \alpha p_g = \left(p_g - \xi \rho_g \left\| \vec{u}_g \right\|^2 \right) \vec{\nabla} \alpha - \lambda \vec{u}_g$$

- **Energy**

$$\frac{\partial \alpha \rho_g E_g}{\partial t} + \vec{\nabla} \cdot \left(\alpha \rho_g E_g \vec{u}_g + \alpha p_g \vec{u}_g \right) + \vec{\nabla} \cdot \alpha \vec{q}_g - \alpha \rho_g \varepsilon_g = \vartheta \left(T_s - T_g \right)$$

$$\frac{\partial (1-\alpha) \rho_s e_s}{\partial t} + \vec{\nabla} \cdot (1-\alpha) \vec{q}_s - (1-\alpha) \rho_s \varepsilon_s = -\vartheta \left(T_s - T_g \right)$$



***R.A. Berry, *Notes on Well-Posed, Ensemble Averaged Conservation Equations for Multiphase, Multi-Component, and Multi-Material Flows*, INL/EXT-05-00516, July 2005.**

Tasks

2. Three-Dimensional Development
    - HPC
    - Mesh Management
    - Visualization
3. Optimization of Physical Models (Turbulence)
4. Validation
    - Known Benchmarks (analytical and numerical)
    - Experiments